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Transport Phenomena in a Plane Shock Wave

A. G. Bashkirov[1] and A. V. Orlov[1]

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With the use of the nonpolynomial closure $1/v_z$ in the Mott-Smith approximation of the solution of the Boltzmann equation, we obtain a value of the density gradient in the limit of a very weak shock wave that is close to the correct value. For the determination of the transverse temperature gradient we calculated the v_x^2/v_z moment of the Mott-Smith collision integral. The effective values of viscosity and thermal conductivity in the limit of a very weak shock wave were calculated for inverse-power potentials and found to agree almost exactly with the Chapman–Enskog values. Such a comparison can serve as a criterion for the evaluation of different bimodal theories. Various bimodal theories give different values of viscosity and thermal conductivity, but all of them give 33% too high a value of the Eucken ratio.

KEY WORDS: Shock wave; Boltzmann equation; Mott-Smith theory; nonpolynomial closure; transverse temperature; viscosity; thermal conductivity.

1. INTRODUCTION

In the Mott-Smith method[1] and in a number of related treatments[2–6] a plane stationary shock wave is described by the bimodal distribution function

$$f_b = \nu(z)\, f_0(\mathbf{v}) + [1 - \nu(z)]\, f_1(\mathbf{v}) \tag{1}$$

where

$$f_i = n_i(2RT_i/\pi)^{-3/2} \exp[-(\mathbf{v} - \mathbf{u}_i)^2/2RT_i]$$

$\nu(+\infty) = 0$, $\nu(-\infty) = 1$, and $n_i, \mathbf{u}_i$, and T_i are upstream $(i = 0)$ and downstream $(i = 1)$ densities, velocities and temperatures, respectively.

[1] 47A-45 Trifonovskaya St, Moscow, 129272, USSR.

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The first three moments of the Boltzmann equation (for 1, v_z, and v^2) give the Hugoniot relations at the discontinuity. For the determination of the function $\nu(z)$ Mott-Smith and other authors suggest using the additional moment closing equation for a polynomial function $\varphi(\mathbf{v})$:

$$\frac{d}{dz}\langle v_z\varphi\rangle_b = \int d^3v\ \varphi J(f_b, f_b)$$

or

$$(\langle v_z\varphi\rangle_0 - \langle v_z\varphi\rangle_1)\, d\nu/dz = \int d^3v\ \varphi[J(f_0, f_1) + J(f_1, f_0)]\ \nu(1-\nu) \quad (2)$$

where $\langle\cdots\rangle_i = \int d^3v \cdots f_i$, $i = b$, 0, 1.

The solution of this equation for any φ is of the form

$$\nu(z) = [1 + \exp(4z/\delta)]^{-1}$$

The shock wave thickness $\delta = 1/|d\nu/dz|_{\max}$ is thus the only quantity that depends on the Mach number M, the intermolecular potential, and the choice of a closing equation.

Various bimodal theories[1-6] have been compared with experiment, but we offer an analytical asymptotic ($M \to 1$) approach to the evaluation of these theories based on the comparison of the effective viscosity and thermal conductivity coefficients calculated by means of the distribution function f_b with the Chapman–Enskog values of these coefficients. This comparison is made in Appendix A. The trimodal approximation of Salwen *et al.*[8] is shown to give the best results. In this paper, however, we shall treat only the bimodal approximation, because of its physical clarity and analytical ease.

In Section 2 we suggest using $1/v_z$ as a closing moment. In Section 3 we use the v_x^2/v_z moment equation for the evaluation of the transverse temperature gradient. We calculate corresponding transport coefficients for several intermolecular potential and for $M \to 1$. Details are given in Appendix B.

2. USING $1/v_z$ CLOSURE

The bimodal distribution function obeys the requirement that its three moments for v_z, v_z^2, and $v_z v^2$ are equal to the corresponding moments of the exact solution of the Boltzmann equation:

$$\langle v_z\rangle_b = \langle v_z\rangle, \qquad \langle v_z^2\rangle_b = \langle v_z^2\rangle, \qquad \langle v_z v^2\rangle_b = \langle v_z v^2\rangle \quad (3)$$

But we cannot say anything about a similar relation for $\langle 1 \rangle_b$, so the use of the bimodal function for the evaluation of the density (or velocity) is completely unjustified.

Nevertheless, it is shown in Appendix A that the v_z^2 closing equation gives the exact limiting value (when $M \to 1$) of the velocity (and hence density) gradients. The success of this closure seems to be a kind of good fortune.

The choice of the moment equation with $1/v_z$ as a closure is more consistent. In the lhs of this equation we have from Eq. (2)

$$(n_0 - n_1)\, dv/dz = (9mn_0^2/32\mu)(5RT_0/3)^{1/2}\alpha^2 v(1-v), \quad \alpha = M^2 - 1 \to 0 \tag{4}$$

where μ is the effective viscosity coefficient (see Appendix A). The collision integral in the lowest approximation is

$$J(f_b, f_b) = \tfrac{1}{2}v(1-v)\int d^3v_1\, |\mathbf{v}_1 - \mathbf{v}|\, b\, db\, d\varepsilon\, f_0(\mathbf{v})\, f_0(\mathbf{v}_1)$$

$$\times (4u^2\{c_z^2\} - 4ut\{c_z c^2\} + t^2\{c^4\})$$

where $u = (u_0 - u_1)/(2RT_0)^{1/2}$, $t = T_1/T_0 - 1$, $\mathbf{c} = (\mathbf{v} - \mathbf{u}_0)/(2RT_0)^{1/2}$, and $\{A\} = A' + A_1' - A - A_1$.

For the integration over ε we pass to the center-of-mass velocity $\mathbf{G} = (\mathbf{c} + \mathbf{c}_1)/2$ and the relative velocity $\mathbf{g} = \mathbf{c}_1 - \mathbf{c}$ and make use of the dependence of $\mathbf{g}'$ on $\mathbf{g}$ cited, e.g., by Bird.[10] After some calculations we obtain

$$J = (\alpha^2 n_0^2/4\pi^2)(2RT_0)^{-3/2} v(1-v)$$

$$\times \int d^3c_1\, |\mathbf{v}_1 - \mathbf{v}|\, b\, db \sin^2\chi \exp(-c^2 - c_1^2)$$

$$\times [(15/8)(g^2 - 3g_z^2) - 3a(G_z g^2 - 3g_z \mathbf{G}\cdot\mathbf{g}) + G^2 g^2 - 3(\mathbf{G}\cdot\mathbf{g})^2] \tag{5}$$

where

$$a = (5/6)^{1/2}$$

At first we restrict ourselves to Maxwell molecules. For this model we have

$$\int |\mathbf{v}_1 - \mathbf{v}|\, b\, db \sin^2\chi = 2kT_0/3\pi\mu_0$$

so in the rhs of Eq. (5) we can integrate over $\mathbf{c}_1$. After that, multiplying by $1/v_z$ and integrating over c_x and c_y, we get

$$\int d^3v\, J/v_z = \xi\alpha^2 n_0^2 (2\pi RT_0)^{-1/2}(2kT_0/3\mu_0)\, v(1-v) \tag{6}$$

where

$$\xi = \int_{-\infty}^{\infty} dc_z\,(c_z + a)^{-1}(3/8 - 9ac_z/8 - 9c_z^2/16 + 3ac_z^3/4 - c_z^4/8)\exp(-c_z^2)$$

The principal value of ξ is

$$\xi = [29a + (17/36)\sqrt{\pi}\exp(-a^2)\operatorname{erfi} a]\sqrt{\pi}/48 = 1.430 \tag{7}$$

Thus, equating the right-hand sides of Eqs. (4) and (6) and taking into account Eq. (7) and the Chapman–Enskog value of μ_0, we obtain for Maxwell molecules (cf. Appendix A)

$$\bar{\mu} = \mu/\mu_0 = 27a\sqrt{\pi}/32\xi = 0.954$$

The calculations for an arbitrary inverse-power potential are carried out in Appendix B.

3. CALCULATION OF THE TRANSVERSE TEMPERATURE GRADIENT AND THE EFFECTIVE THERMAL CONDUCTIVITY

The bimodal function f_b does not satisfy any conditions similar to (3) for the moment $\langle v_x^2 \rangle$. That is why the calculation of the transverse temperature $T_x = \langle mv_x^2 \rangle / kn$ with the use of f_b is not correct. But that is exactly what was done in all the bimodal theories,[1-7] leading to too high values of κ (see Appendix A), i.e., to too low temperature gradients.

To estimate the transverse temperature gradient, we propose to apply the v_x^2/v_z moment equation:

$$d\langle v_x^2 \rangle/dz = \int d^3v\, J(f_b, f_b)\, v_x^2/v_z \tag{8}$$

Here f_b is supposed to be determined with v_z^2 closure, or with $1/v_z$ closure, as these closures provide the correct density gradient. The lhs of Eq. (8) is $n(z)\, dT_x/dz + T_x\, dn/dz$.

With the use of Eq. (5), the rhs of Eq. (8) for Maxwell molecules takes the form

$$\int d^3v\, Jv_x^2/v_z = \zeta \alpha^2 n_0^2 (2\pi R T_0)^{1/2} (2kT_0/3\pi\mu_0)\, \nu(1-\nu)$$

where

$$\zeta = \frac{1}{8}\int_{-\infty}^{\infty} dc_z\,(c_z + a)^{-1}(31/8 - 3ac_z/2 - 13c_z^2/4 + 3ac_z^3 - c_z^4/2)\exp(-c_z^2)$$

$$= [77a - \sqrt{\pi}\exp(-a^2)\operatorname{erfi} a]\sqrt{\pi}/96 = 1.294$$

If we determine $n(z)$ using the Mott-Smith theory with v_z^2 closure, we then obtain from Eq. (8)

$$(dT_x/dz)_{M\to 1, z=0} = 0.0288\alpha^2(n_0 m^2/k\mu_0)(2RT_0)^{3/2}$$

For the calculation of the average temperature gradient we use T_z given by f_b determined by v_z^2 closure. Thus, we obtain

$$\kappa = 1.08\kappa_0$$

where κ_0 is the Chapman–Enskog value. We may as well use f_b determined by $1/v_z$ closure. In this case we have

$$\kappa = 1.11\kappa_0$$

Similar calculations for non-Maxwell inverse-power potentials are made in Appendix B.

4. CONCLUSIONS

We suggested using a nonpolynomial closure for the Mott-Smith approximation. With the use of $1/v_z$ closure and v_x^2/v_z for the determination of the transverse temperature gradient, we calculated the effective values of viscosity and thermal conductivity for inverse-power potentials (from Maxwell molecules to rigid spheres) and found that they are close enough to the Chapman–Enskog values when $M \to 1$. All known bimodal theories were thus evaluated and were found to give the same 33 % too high value of the Eucken ratio.

APPENDIX A

The Mott-Smith approximation function is a linear combination of two Maxwellians. That is why it is easy to calculate with this distribution function the profiles of density, velocity, pressure, viscous stress and heat flux, longitudinal and transverse temperatures, and their gradients. Some of these calculations were made by Mott-Smith[1] and Bird.[10] In the limit $M \to 1$ we can thus obtain the effective viscosity μ as the ratio of the viscous stress to the velocity gradient

$$\mu = (\delta/8)\, m(u_0 - u_1)\, n(z)|_{M\to 1}$$

and the effective thermal conductivity as the ratio of the heat flux to the temperature gradient

$$\kappa = (\delta/4) m n_0 u_0 R(u_0 - u_1)/\{(u_0 + u_1)/5 + (u_0 - u_1)[n_0(z) - n_1(z)]/3n(z)\}|_{M\to 1}$$

Table I. Reduced Viscosity and Thermal Conductivity for Various Shock Wave Theories[a]

	$\bar{\mu}$	$\bar{\kappa}$	Δ	$\bar{\kappa}_{\bar{\mu}}$	$\Delta_{\bar{\mu}}$
Ref. 1, v_z^2	1	4/3	0.33	1.084; 1.126*	0.08; 0.12*
Ref. 1, v_z^3	7/6*	14/9*	0.58*	1.042*	0.17*
Ref. 2	47/90*	94/135*	0.57*	2.321*	1.40*
Refs. 3 and 5	3/5	4/5	0.45	1.698; 1.802*	0.73; 0.83*
Ref. 4	0.957*	1.275*	0.28*	1.155*	0.16*
Ref. 6	10/13	40/39	0.23	1.354	0.42
Ref. 8, v_z^2, v_z^3	1	68/71	0.04	1.126	0.13
Ref. 8, v_z^2, $v_z v^2$	1	1	0	1.126	0.13
Ref. 8, v_z^3, $v_z v^2$	163/160	41/40	0.03	1.114	0.12
Present work, $1/v_z$	0.954; 1.086*	1.272; 1.448*	0.28; 0.46*	1.113; 1.076*	0.12; 0.11*

[a] Maxwell molecules and/or rigid spheres (asterisk).

The comparison of these effective transport coefficients with their Chapman–Enskog counterparts permits us to compare various bimodal theories. The results are presented in Table I in the form of reduced coefficients $\bar{\mu} = \mu/\mu_0$ and $\bar{\kappa} = \kappa/\kappa_0$. Note that various bimodal theories give more or less satisfactory μ and κ, but all of them give the same 33% too high value of the Eucken ratio.

As long as the viscous stress does not depend explicitly on the closure,[10] Table I shows that the Mott-Smith theory for $\varphi = v_z^2$ describes the shock wave thickness and the gradient of the density (as well as of the velocity) correctly in the limit $M \to 1$! For bigger M this theory gives a thickness δ well describing the Monte Carlo simulation results.[10–12] As a general estimation parameter, we introduced Δ:

$$\Delta^2 = (\bar{\mu} - 1)^2 + (\bar{\kappa} - 1)^2$$

The results of the trimodal theory of Salwen *et al.*[8] for various pairs of closing moments are also presented in Table I for completeness. The last two columns of Table I present the thermal conductivity $\bar{\kappa}_{\bar{\mu}}$ and the corresponding value of $\Delta_{\bar{\mu}}$ calculated for Maxwell molecules and/or for rigid spheres (denoted by an asterisk) with the use of the method of Section 3 and $\bar{\mu}$ obtained in each reference.

APPENDIX B

For the calculation of the effective viscosity in the limit $M \to 1$ for the intermolecular potential $U \sim r^{-p}$ we use Eqs. (4)–(6) to obtain, after the transformation $\sqrt{2}\,\mathbf{G} \to \mathbf{G}$, $\mathbf{g}/\sqrt{2} \to \mathbf{g}$,

$$\bar{\mu}^{-1} = [9\sqrt{5/3}\,\pi^{5/2}\Gamma(4-2/p)/10]^{-1}$$
$$\times \int d^3G\, d^3g\, [G_z + \sqrt{5/3} - g_z]^{-1} g^{1-4/p}$$
$$\times \exp(-G^2 - g^2)[(15/4)(g^2 - 3g_z^2)$$
$$- 3\sqrt{5/3}\,(G_z g^2 - 3g_z \mathbf{G}\cdot\mathbf{g}) + G^2g^2 - 3(\mathbf{G}\cdot\mathbf{g})^2]$$

The integration over G_x, G_y and over G_z in the sense of the principal value is carried out easily. After that we use the identity

$$\int_{-\infty}^{\infty} dg_x \int_{-\infty}^{\infty} dg_y\, f(g, g_z) = 2\pi \int_{|g_z|}^{\infty} dg\, g f(g, g_z)$$

for integration over g_x, g_y. The remaining integral over g_z

$$\bar{\mu}^{-1} = [10\sqrt{\pi}/9h\Gamma(4-2/p)]$$
$$\times \int_{-\infty}^{\infty} dg_z\, (\Gamma_5 - 3g_z^2\Gamma_3)(g_z^2 - 5hg_z + 119/12)$$
$$\times \exp(-b^2)\,\mathrm{erfi}\, b$$

where $b = h - g_z$, $h = \sqrt{5/3}$, and $\Gamma_N = \Gamma(N/2 - 2/p, g_z^2)$, was computed on a PC using the Hermite quadrature formula. The results are presented in Table II.

For the calculation of the effective thermal conductivity we first express the longitudinal temperature gradient in terms of μ with the use of Eq. (4) and the transverse temperature gradient in terms of the integral (8). The ratio of the heat flux to the gradient of the average temperature gives the effective thermal conductivity. After some algebra we have

$$(1/\bar{\kappa} + 1/2\bar{\mu})\, \nu(1-\nu)(3/8)\, h\alpha^2 n_0^2 m(RT_0)^{3/2}/\mu_0 = \int d^3v\, Jv_x^2/v_z$$

Table II. Reduced Viscosity and Thermal Conductivity for the Inverse-Power Potential $U \sim r^{-p}$

p	4	5	6	7	8	10	11	∞
$\bar{\mu}$	0.954	0.978	0.994	1.006	1.016	1.029	1.034	1.086
$\bar{\kappa}_1$	1.084	1.092	1.097	1.102	1.104	1.108	1.110	1.126
$\bar{\kappa}_2$	1.113	1.104	1.099	1.096	1.093	1.089	1.088	1.076
Δ_1	0.08	0.09	0.10	0.10	0.10	0.11	0.11	0.13
Δ_2	0.12	0.11	0.10	0.10	0.09	0.09	0.09	0.11

The integration in the rhs is carried out in the same way as before. The result is

$$\begin{aligned}1/\bar{\kappa}+1/2\bar{\mu}= & -8/9+[5\sqrt{\pi}/12h\Gamma(4-2/p)]\\ & \times\int_{-\infty}^{\infty} dg_z\,[(13/4-3hb+b^2)(\Gamma_7-4g_z^2\Gamma_5+3g_z^4\Gamma_3)\\ & +(11/4+3hb+b^2)(\Gamma_5-3g_z^2\Gamma_3)-g_z(9h+6b)(\Gamma_5-g_z^2\Gamma_3)]\\ & \times\exp(-b^2)\,\mathrm{erfi}\,b\end{aligned}$$

This expression for $\bar{\kappa}$ was used with v_z^2 closure, when $\bar{\mu}=1$ ($\bar{\kappa}_1$), and with $1/v_z$ closure ($\bar{\kappa}_2$). The results are also presented in Table II.

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